Effects of interwall interaction on the electrical conductance at the junction between a double-walled carbon nanotube and copper electrodes

Feng Gao,[1] Jianmin Qu,[1,2,a)] and Matthew Yao[3]
[1]*Department of Civil and Environmental Engineering, Northwestern University, Evanston, Illinois 60208, USA*
[2]*Department of Mechanical Engineering, Northwestern University, Evanston, Illinois 60208, USA*
[3]*Rockwell Collins Inc., Cedar Rapids, Iowa 52498, USA*

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Considered in this letter are the effects of interwall interaction on the electrical conductance at the junction of a double-walled carbon nanotube (DWCNT) between two copper electrodes. In the end-contact configuration, the effect of interwall interaction on the electrical conductance is rather weak, and both walls of DWCNT contribute to the electronic transport almost as if they are parallel connectors. In the side-contact configuration, not only the inner tube does not contribute to the overall electrical conductance, its presence hinders the electronic transport of the outer wall by causing significant localization of density of states near the Fermi level. © *2011 American Institute of Physics*. [doi:10.1063/1.3582242]

Metals, such as copper (Cu), have been the de facto materials for electrical interconnect in semiconductor devices. However, as the line width in semiconductors decreases to nanometer scales, electrical conductivity in metallic interconnects starts to degrade due to increased grain boundary and surface scattering.[1] Carbon nanotube (CNT) on the other hand has long electron mean free path ($>1\ \mu$m) and can carry very high current density ($>10^9\ \text{A/cm}^2$).[2–6] Due to these excellent electrical properties, CNTs are considered a promising material for electrical interconnects in microscale and nanoscale electric devices.[7,8]

Multiwalled CNTs (MWCNTs) are often formed during the CNT growth process. MWCNTs are mostly metallic because of their large diameter and multiple walls. Vertical MWCNT interconnects have already been investigated for conducting vias, and for through-wafer-three-dimensional interconnects. The ability to estimate the electrical conductance of the MWCNT is critical in such applications. Electrical conductance of single-walled CNTs (SWCNTs) near the CNT/Cu junction has been studied previously by the Gao *et al.*[9,10] and others.[11–13] However, due to the discrete nature of the MWCNT, it is perceivable that the electrical conductivity of MWCNT may not be the same as the SWCNT because of the interwall interactions. It is thus important to understand how the interwall interactions take place and how such interaction affects the overall electrical conductance of the CNT/Cu junction. Although the electrical conductance of MWCNT itself has been studied both experimentally and numerically,[5–8,14,15] electrical conductance at MWCNT/Cu junction has not been studied yet.

In this letter, we investigated the interaction between the walls on the electrical conductance at MWCNT/Cu junctions by using quantum mechanics calculations. Considered in this study are two types of commonly used MWCNT/Cu junctions, end contact and side contact as illustrated in Fig. 1. Figure 1(a) shows the end-contact configuration where a double-walled CNT (DWCNT) is in contact with a Cu electrode at each end, while Fig. 1(b) shows the side contact configuration where two Cu electrodes are juxtaposed in contact with the outer wall of a DWCNT. The DWCNT considered here consists of two metallic SWCNTs, whose chirality are (5,5) and (10,10), respectively. This is one of the most stable configurations for armchair DWCNT.[16] The distance between the walls is 3.39 Å, which is almost the same as the

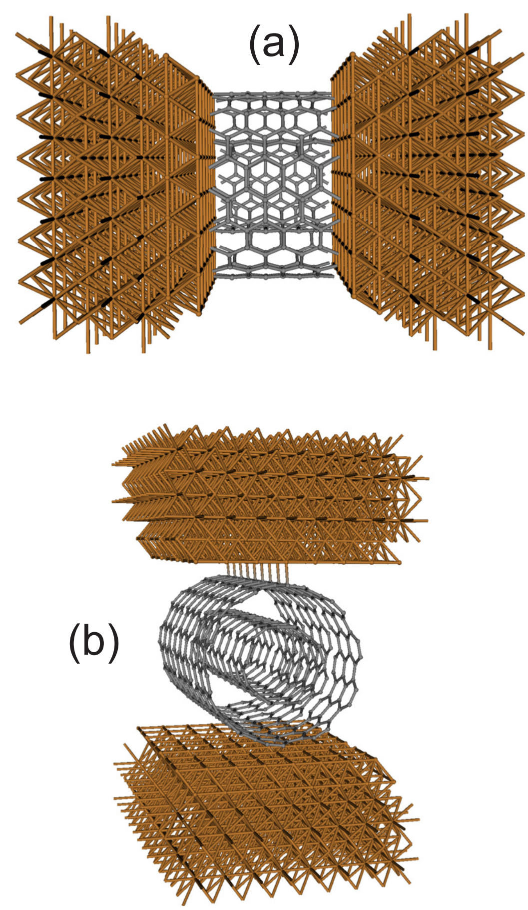

FIG. 1. (Color online) The DWCNT/Cu junction configurations: (a) end contact and (b) side contact: the inner tube of DWCNT is (5,5) while the outer tube is (10,10).

a)Electronic mail: j-qu@northwestern.edu.

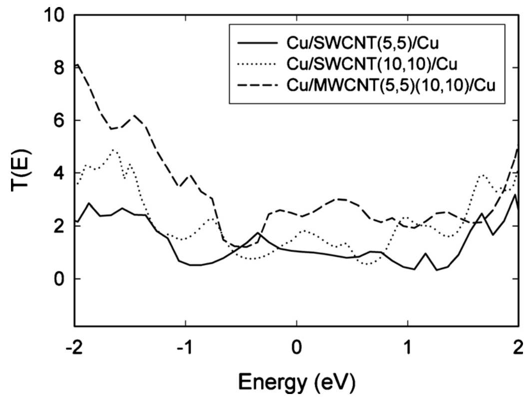

FIG. 2. The electron transmission spectrum of end-contact Cu/CNT/Cu junction: the solid line is for Cu/SWCNT(5,5)/Cu, the dotted line is for Cu/SWCNT(10,10)/Cu, and the long-dash line is for Cu/DWCNT(5,5@10,10)/Cu.

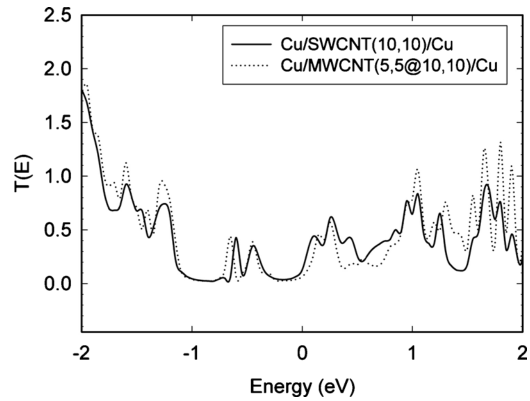

FIG. 3. The electron transmission spectrum of side-contact Cu/SWCNT/Cu and Cu/DWCNT/Cu systems.

experimentally observed wall-to-wall distance of 3.4 Å, as well as interlayer spacing in graphite.[16,17]

In the side-contact configuration shown in Fig. 1(b), the lattice structure of Cu electrode has been stretched slightly (~3% strain) so that its length matched that of the CNT. This is necessary in order to avoid C–C dangling bond at the CNT ends when periodic boundary conditions are used in the tube axis direction.

In both configurations, the distance between the CNT and Cu electrode is determined by minimizing the total energy of the system.[9] As a comparison, the SWCNT/Cu results are also presented.

To calculate the electrical conductance, a steady-state electrical current is induced in the Cu/DWCNT/Cu junction by applying a bias voltage between the two Cu electrodes. All calculations were performed based on the generalized gradient approximation with the Perdew–Burke–Ernzerhof pseudoatomic potentials. The k-point sampling in the Brillouin zone integration parameters is 5, 5, and 100 in x-, y-, and z-directions, respectively. The basis set double-zeta was utilized in this study. The energetic convergence criterion for the Hamiltonian, charge density, and band-structure energy is 1×10^{-5}.

The electron transmission across the Cu/DWCNT/Cu junctions is calculated by using the nonequilibrium Green's function method within the density functional theory framework.[10] Figure 2 shows the calculated electron transmission spectrums of the DWCNT/Cu system in end contact. The long-dashed solid line is for the DWCNT, and the solid and dotted lines are for SWCNT of (5,5) and (10,10), respectively. It is seen that the electron transmission coefficient for the DWCNT is greater than that of the SWCNTs, particularly in the vicinity of Fermi level. In other words, both the inner and outer tubes in the DWCNT participated in the electron transport.

To compute the junction electrical resistance, the I-V relationship of the Cu/DWCNT/Cu system is needed. This can be obtained by using the Landauer–Buttiker formula, which relates the conductance to the transmission probability $T(E,V)$,[10]

$$I(V) = \frac{2e}{h}\int_{\mu_1}^{\mu_2} dE\,T(E,V)[f(E-\mu_1)-f(E-\mu_2)], \qquad (1)$$

where μ_1 and μ_2 are the chemical potentials of left and right electrodes, $f(E-\mu)=1/\{1+\exp[E-\mu/k_BT_{\mathrm{temp}}]\}$ is the Fermi–Dirac distribution function, k_B is the Boltzmann constant, T_{temp} is the temperature, and $T(E,V)$ is the transmission function. The transmission function can be calculated through the independent $\mathbf{k}_\parallel$ (surface-parallel direction reciprocal lattice vector point) channels and their integral over the two-dimensional reciprocal unit cell.[10]

Once the I-V relationship is known, the total resistance of the system can be computed via the Ohmic law by averaging the values between 0 and 0.1 V. The total resistance of the end-contact Cu/DWCNT/Cu junction is found to be 5.43 kΩ. The values for Cu/SWCNT(5,5)/Cu and Cu/SWCNT(10,10)/Cu systems are 12.00 kΩ and 9.03 kΩ, respectively. Should there be no interwall interaction at all, the DWCNT can be considered as two separate SWCNT connecting the electrodes, and the total resistance would be 5.14 kΩ. The fact that the junction resistance of the DWCNT is 5.43 kΩ (slightly higher than that of two separate SWCNT) indicates that there is a weak interwall interaction which slightly hinders the electron transports in the axial direction.

Results for the side contact, however, are quite different. Shown in Fig. 3 are the comparison electron transmission spectrum for the Cu/SWCNT(10,10)/Cu system and the Cu/DWCNT/Cu in side contact. The similarity between these two cases implies that the electron transmission in the DWCNT is primarily through the outer wall. Further, our results show that the total electrical resistance of the Cu/DWCNT/Cu is 71.4 kΩ, while that of the Cu/SWCNT(10,10)/Cu system is only 57.9 kΩ. In other words, the presence of the inner wall (5,5) reduces the electrical conductance of the outer wall by more than 20%. Clearly, the interwall interaction in this case is much more detrimental to the electrical conductance.

The interwall interaction in DWCNT has been studied based on the charge distribution.[18,19] It was found that the accumulated charge density in the region between the walls reduces the electrical conductance of the outer wall. In addition, Miyamoto *et al.*[18] have reported that the interwall interactions shift the electron density slightly from the outside of the SWCNT to the region between the two tubes, thus one would expect a slight decrease in the conductance of the DWCNT compared to the SWCNT.[19] Our results for both end and side contact systems show that interwall interaction also reduces the electrical conductance of Cu/DWCNT/Cu systems compared to Cu/SWCNT/Cu system. Furthermore,

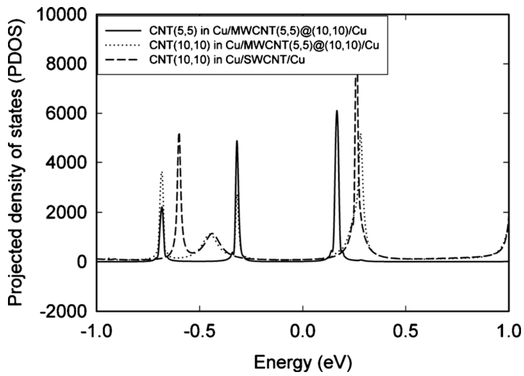

FIG. 4. PDOS of individual tubes in side-contact Cu/SWCNT(10,10)/Cu and Cu/DWCNT(5,5@10,10)/Cu systems.

such interaction is much stronger in side contact than in end contact.

To understand why the interwall interaction is much stronger in side contact, we plotted the projected density of states (PDOS) in Fig. 4 for the side contact configurations. The solid line and the dotted line are, respectively, the PDOS of the inner and outer tubes in the Cu/DWCNT/Cu junction, while the long-dashed lines is the PDOS of the Cu/SWCNT(10,10)/Cu junction. If there were no interwall interaction, the dished line and dotted line should be the same. The fact that the dotted line shows additional DOS peaks near the Fermi level is a clear indication of the interwall interaction. We note that the inner tube (5,5) in the DWCNT is localized around −0.3 eV. This causes the DOS of the outer tube (10,10) to localize at the same energy level as well. Such DOS localization near the Fermi level is the main reason for the reduced electrical conductance. On the other hand, we find that the PDOS for the end-contact configuration does not show such strong localization, indicating that both the inner tube (5,5) and the outer tube (10,10) act as if they are SWCNTs in parallel without significant interaction.

In summary, effects of interwall interaction on the electrical conductance at Cu/DWCNT/Cu junctions are investigated in this study. It is found that, in the end-contact configuration, the effect of interwall interaction on the total electrical conductance is rather weak, and both walls of the DWCNT contribute to the electron transport almost as if they are parallel connectors. In the side-contact configuration, not only the inner tube does not contribute to the overall electrical conductance, its presence severally hinders the electronic transport ability of the outer wall by causing significant localization of the density of states near the Fermi level.

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